Universal renormalization of saddle-point integrals for condensed Bose gases

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(Received 2 March 1999)

When treating the ground-state contribution exactly, a variant of the saddle-point method emerges that works even for condensed Bose gases. Results thus obtained, such as canonical partition functions, differ by universal renormalization factors from those provided by the conventional but incorrect scheme. The amended method yields the statistical properties of ideal and very weakly interacting Bose gases with a fixed number of particles with particular simplicity. [S1063-651X(99)13012-5]

PACS number(s): 05.30.Ch, 05.30.Jp, 03.75.Fi

The saddle-point method [1] is one of the true work horses of statistical mechanics. Greatly promoted by Schrödinger's lucid discussion [2], it serves as *the* essential tool for the comparison of different statistical ensembles. In the field of Bose-Einstein condensation, however, this work horse shows signs of illness, which already thwarts the attempt to compute canonical partition functions of ideal Bose gases [3]. As detailed below, the usual answer to this textbook problem [4], probably given by generations of physicists, turns out to be *incorrect* in the condensate regime; moreover, the standard saddle-point approximation does not yield the correct fluctuation of the number of condensate particles [5,6]. This shortcoming is particularly painful since there is now, in the wake of the impressive series of successful experiments on atomic Bose-Einstein condensates [7], enhanced interest in the statistical mechanics of mesoscopically small, isolated samples of Bosons [8–11] which cannot be described by the customary grand canonical ensemble.

In this paper we discuss the reason for the failure of the standard approach, and modify the saddle-point approximation such that it works for *all* temperatures. The correct canonical N-particle partition functions will then allow us to demonstrate the large-N equality of grand canonical and canonical occupation numbers also in the condensate regime and to assess the sharpness of the onset of Bose-Einstein condensation in a gas with a fixed, finite number of particles. Comparing the results of the standard saddle-point scheme to those provided by the properly amended one, it is found that the error of the former is *universal*, that is, independent of the system's single-particle spectrum, so that correct results can be obtained even from the standard scheme by means of a simple, multiplicative renormalization.

We start from the familiar expansion [4] of the grand canonical partition function $\Xi(\beta,z)$ of an ideal Bose gas with single-particle energies ε_ν $(\nu=0,1,2,\ldots)$ in terms of the canonical partition functions $Z_N(\beta)$,

$$\Xi(\beta,z)=\prod_{\nu=0}^{\infty}\frac{1}{1-z\exp(-\beta\varepsilon_\nu)}=\sum_{N=0}^{\infty}z^N Z_N(\beta), \tag{1}$$

where $\beta=1/(k_BT)$ is the inverse temperature. Hence, writing $\Xi(\beta,z)/z^{N+1}\equiv\exp[-\overline{F}_1(z)]$, or

$$\overline{F}_1(z)=(N+1)\ln z+\sum_{\nu=0}^{\infty}\ln(1-ze^{-\beta\varepsilon_\nu}),$$

the desired N-particle partition function $Z_N(\beta)$ is extracted from this series (1) by means of a contour integral

$$Z_N(\beta)=\frac{1}{2\pi i}\oint dz\,\exp[-\overline{F}_1(z)], \tag{2}$$

where the path of integration encircles the origin of the complex z plane counterclockwise. The saddle point z_1 is then determined from the requirement that the logarithm of the integrand becomes stationary, i.e., from $\partial\overline{F}_1(z)/\partial z|_{z=z_1}=0$. This yields the relation

$$N+1=\sum_{\nu=0}^{\infty}\frac{1}{z_1^{-1}e^{\beta\varepsilon_\nu}-1}, \tag{3}$$

which looks like a grand canonical equation for the fugacity z_1 in a gas with $N+1$ bosons. Now one relies on the fact that for large N the main contribution to the integral (2) is collected in the neighborhood of the saddle point [2], leads the contour parallel to the imaginary axis over the saddle, and usually employs the Gaussian approximation

$$\begin{aligned}\tilde{Z}_N(\beta)&=\frac{1}{2\pi i}\int_{z_1-i\infty}^{z_1+i\infty}dz\,\exp\left[-\overline{F}_1^{(0)}-\frac{1}{2}\overline{F}_1^{(2)}(z-z_1)^2\right]\\&=(-2\pi\overline{F}_1^{(2)})^{-1/2}\exp(-\overline{F}_1^{(0)}),\end{aligned} \tag{4}$$

where $\overline{F}_1^{(n)}$ is the nth derivative of $\overline{F}_1$ at z_1, so that

$$\overline{F}_1^{(2)}=-\sum_{\nu=0}^{\infty}\frac{z_1^{-1}e^{-\beta\varepsilon_\nu}}{(1-z_1e^{-\beta\varepsilon_\nu})^2}. \tag{5}$$

Within this approximation (4), the logarithm of the canonical N-particle partition function reads

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$$\ln \tilde{Z}_N(\beta) = -(N+1)\ln z_1 - \sum_{\nu=0}^{\infty} \ln(1 - z_1 e^{-\beta\varepsilon_\nu}) - \frac{1}{2}\ln 2\pi - \frac{1}{2}\ln\sum_{\nu=0}^{\infty} \frac{z_1^{-1} e^{-\beta\varepsilon_\nu}}{(1 - z_1 e^{-\beta\varepsilon_\nu})^2}, \qquad (6)$$

from which the canonical occupation number $\langle n_\alpha \rangle_{\rm cn}$ of the single-particle state with energy ε_α is obtained by differentiating once with respect to $-\beta\varepsilon_\alpha$,

$$\langle n_\alpha \rangle_{\rm cn} = \frac{\partial \ln \tilde{Z}_N}{\partial(-\beta\varepsilon_\alpha)} + \frac{\partial \ln \tilde{Z}_N}{\partial z_1} \frac{\partial z_1}{\partial(-\beta\varepsilon_\alpha)}. \qquad (7)$$

For temperatures above the onset of Bose condensation, the second sum on the right-hand side of Eq. (6) can be neglected against the first. Then $\partial \ln \tilde{Z}_N / \partial z_1$ vanishes as a consequence of the saddle-point equation (3), so that

$$\langle n_\alpha \rangle_{\rm cn} = \frac{\partial \ln \tilde{Z}_N}{\partial(-\beta\varepsilon_\alpha)} = \frac{1}{z_1^{-1} e^{\beta\varepsilon_\alpha} - 1}. \qquad (8)$$

Thus, for the large N considered these occupation numbers equal their grand canonical counterparts [4].

However, in the condensate regime the situation is quite different, since there the sum in Eq. (3) is dominated by the ground-state contribution, so that $z_1^{-1} e^{\beta\varepsilon_0} - 1$ is on the order of $1/N$. Then both sums in Eq. (6) are of the *same* order $O(\ln N)$, and the neglect of the second is no longer justified. Even worse, the entire saddle-point approximation (4) breaks down [3]. The Gaussian integral (4) can capture the behavior of the exact partition function (2) only if $\overline{F}_1(z)$ is free of singularities in those intervals where the approximation gathers its major contributions, that is, for those z where $\overline{F}_1^{(2)}(z - z_1)^2$ is on the order of unity. Since $\overline{F}_1^{(2)} = O(N^2)$ by Eq. (5), the familiar saddle-point scheme (4) can produce correct results *only* if $\overline{F}_1(z)$ remains regular at least in an interval of order $O(1/N)$ around z_1. But it does not: Again by Eq. (3), it is just the very hallmark of Bose-Einstein condensation that the saddle-point z_1 approaches the ground-state singularity at $z = e^{\beta\varepsilon_0}$ within order $O(1/N)$. With this diagnosis, the workhorse really is seriously ill.

Fortunately, there is a cure which almost suggests itself. Since it is only the ground state which is causing the trouble, one has to exempt the ground-state contribution to $\overline{F}_1(z)$ from the Gaussian approximation, and to treat that contribution exactly. More precisely, defining

$$F_1(z) = \overline{F}_1(z) - \ln(1 - z e^{-\beta\varepsilon_0}), \qquad (9)$$

the partition functions (2) acquire the still exact form

$$Z_N(\beta) = \frac{1}{2\pi i} \oint dz \frac{\exp[-F_1(z)]}{1 - z e^{-\beta\varepsilon_0}}.$$

If one now lets the dangerous denominator stand as it is, and expands only the ground-state-amputated function $F_1(z)$ quadratically around z_1, then the singular point produced by the first excited state at $z = e^{\beta\varepsilon_1}$ decides the fate of this approximation. Since the saddle point remains pinned below $e^{\beta\varepsilon_0}$, there is a gap wider than $e^{\beta\varepsilon_1} - e^{\beta\varepsilon_0} \approx (\varepsilon_1 - \varepsilon_0)/(k_B T)$ between z_1 and the decisive singularity. For sufficiently large N, this gap hosts an interval on the order of the inverse square root of $-F_1^{(2)}$ around z_1, which is what is required to validate the approximation. Doing the integral [12,13], one arrives at

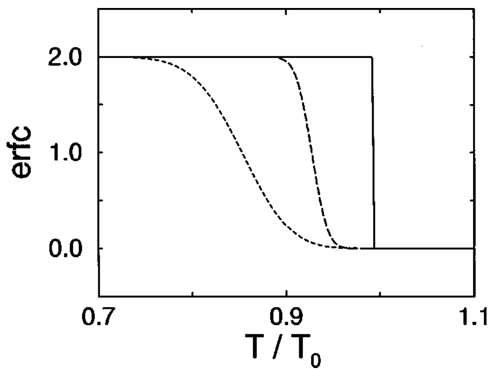

FIG. 1. Complementary error function erfc($\overline{\eta}/\sqrt{2}$) appearing in the canonical partition function (10), for gases of 10^2 (short dashes), 10^3 (long dashes), and 10^6 (full line) ideal Bosons in a three-dimensional isotropic harmonic trap.

$$Z_N(\beta) = \exp\left(\beta\varepsilon_0 - F_1^{(0)} - 1 + \frac{1}{2}\eta^2\right) \frac{1}{2} {\rm erfc}\left(\frac{\overline{\eta}}{\sqrt{2}}\right) \qquad (10)$$

with $\eta = (e^{\beta\varepsilon_0} - z_1)\sqrt{-F_1^{(2)}}$ and $\overline{\eta} = \eta - 1/\eta$. This approximation to the canonical partition functions holds for *all* temperatures. The special treatment of the ground-state contribution is essential in the condensate regime, but for high T, where z_1 stays away from $e^{\beta\varepsilon_0}$, it does not matter whether or not it is included in the Gaussian approximation. Indeed, since both η and $\overline{\eta}$ are large for high T, Eq. (10) then actually reduces to the familiar result (4), $Z_N(\beta) \sim \tilde{Z}_N(\beta)$ in the high-T domain [13]. The most characteristic feature of the partition function (10) now is the appearance of the complementary error function erfc: Its argument drops from large positive numbers at high T to large negative numbers in the condensate regime, so that the steepness of this function quantifies the sharpness of the onset of Bose-Einstein condensation within the canonical ensemble. This finding is illustrated in Fig. 1 for ideal N-particle Bose gases with ''small'' and ''large'' N in a three-dimensional isotropic harmonic oscillator potential. In this and the following figures, the reference temperatures $k_B T_0 = \hbar\omega[N/\zeta(3)]^{1/3}$ correspond to the condensation temperatures in the large-N limit; ω is the oscillator frequency.

In the condensate regime, where $\eta \approx 0$, one finds

$$Z_N(\beta) = \exp(\beta\varepsilon_0 - F_1^{(0)} - 1), \qquad (11)$$

so that the treacherous Eq. (6) is replaced by

$$\ln Z_N(\beta) = \beta\varepsilon_0 - 1 - (N+1)\ln z_1 - \sum_{\nu=1}^{\infty} \ln(1 - z_1 e^{-\beta\varepsilon_\nu}).$$

Evaluating $\partial \ln Z_N / \partial z_1$, the amended Eq. (7) then reads

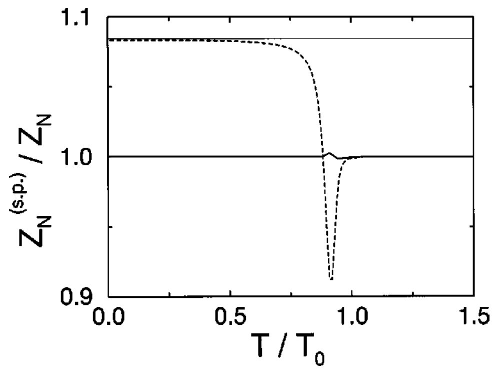

FIG. 2. Ratio of the proper saddle-point approximation (10) (heavy full line) and of the standard ''approximation'' (4) (dashed line) to the exact partition functions, for 10^3 ideal Bosons in a three-dimensional isotropic harmonic trap. The thin line indicates the universal factor $1/R_1 \approx 1.08444$, by which the standard formula fails in the condensate regime. The approximations are denoted as $Z_N^{(\mathrm{s.p.})}$; the exact data for Z_N have been computed recursively [8–10].

$$\langle n_\alpha \rangle_{\mathrm{cn}} = \frac{\partial \ln Z_N}{\partial(-\beta\varepsilon_\alpha)} - \frac{z_1^{-1}}{z_1^{-1} e^{\beta\varepsilon_0} - 1} \frac{\partial z_1}{\partial(-\beta\varepsilon_\alpha)}.$$

Now one has to distinguish two cases: Since $z_1 = e^{\beta\varepsilon_0} + O(1/N)$, one may justly neglect the second term on the right-hand side, as one did in the incorrect reasoning based on Eq. (7), only for $\alpha \neq 0$, and then recovers, and thus validates, Eq. (8). In the case of the ground state, however, the second term is *essential*, yielding

$$\langle n_0 \rangle_{\mathrm{cn}} = -1 - \frac{z_1^{-1}(-e^{\beta\varepsilon_0})}{z_1^{-1} e^{\beta\varepsilon_0} - 1} = \frac{1}{z_1^{-1} e^{\beta\varepsilon_0} - 1}. \qquad (12)$$

This is, of course, an expected result — large-N equality of grand canonical and canonical occupation numbers holds also for the ground state — but it is enlightening to see how the previously ill-famed saddle-point method, if executed properly, manages to do the job: Although the result obtained in Eq. (12) looks similar to Eq. (8) with $\alpha = 0$, the underlying reasoning is distinctly different.

A surprising discovery is made upon trying to reconcile the proper approximation (11) with the standard formula (4). Utilizing the definition (9), and exploiting that $\overline{F}_1^{(2)} \approx -(e^{\beta\varepsilon_0} - z_1)^{-2}$ in the condensate regime, the right-hand side of Eq. (11) becomes

$$Z_N(\beta) = (e^{\beta\varepsilon_0} - z_1)\exp(-\overline{F}_1^{(0)} - 1) \approx \frac{\sqrt{2\pi}}{e} \tilde{Z}_N(\beta),$$

so that that the standard formula (4), while correct at high T, fails in the condensate regime by merely the temperature-independent factor $R_1 = \sqrt{2\pi}/e \approx 0.92214$, regardless of the system's single-particle spectrum, that is, of the trapping potential which confines the gas. This finding, verified in Fig. 2 for $N = 1000$ ideal Bosons in an isotropic harmonic trap, explains why — fortuitously — correct results can be obtained by taking derivatives of the incorrect $\ln \tilde{Z}_N(\beta)$: The error, committed unknowingly, drops out when N is large enough.

Generalizing, we now introduce the quantities

$$I_\sigma = \frac{1}{2\pi i} \oint dz \frac{\exp[-F_\sigma(z) - (\sigma - 1)\beta\varepsilon_0]}{(1 - z e^{-\beta\varepsilon_0})^\sigma}$$

with positive integer σ, and

$$F_\sigma(z) = (N + 2 - \sigma)\ln z + \sum_{\nu=1}^{\infty} \ln(1 - z e^{-\beta\varepsilon_\nu}),$$

so that $Z_N(\beta) \equiv I_1$; moreover, $\langle n_0 \rangle_{\mathrm{cn}}$ is exactly equal to I_2/I_1. The corresponding saddle-point equations

$$N + 2 - \sigma = \frac{\sigma}{z_\sigma^{-1} e^{\beta\varepsilon_0} - 1} + \sum_{\nu=1}^{\infty} \frac{1}{z_\sigma^{-1} e^{\beta\varepsilon_\nu} - 1}, \qquad (13)$$

mimic grand canonical systems with $N + 2 - \sigma$ particles and σ-fold degenerate ground states: The best possible saddle-point calculation of $\langle n_0 \rangle_{\mathrm{cn}}$, more accurate than the approximation (12), formally involves ground-state doubling [13].

The mean-square condensate fluctuations then become

$$\langle \delta^2 n_0 \rangle_{\mathrm{cn}} = I_2/I_1 - (I_2/I_1)^2 + 2I_3/I_1. \qquad (14)$$

Here, the third term acts as a switch: $I_3/I_1 \sim \langle n_0 \rangle_{\mathrm{cn}}^2$ for temperatures above the condensation point, so that then $\langle \delta^2 n_0 \rangle_{\mathrm{cn}} = \langle n_0 \rangle_{\mathrm{cn}} + \langle n_0 \rangle_{\mathrm{cn}}^2$, as in the grand canonical ensemble [4]. In contrast, $2I_3/I_1 \to N^2 - N$, and therefore $\langle \delta^2 n_0 \rangle_{\mathrm{cn}} \to 0$, for $T \to 0$. Following the same amended saddle-point strategy that has already led to the canonical partition function (10), the integrals I_σ can be expressed in terms of parabolic cylinder functions [12,13]. In the condensate regime, we find

$$I_\sigma = \left(\frac{\sigma}{e^{\beta\varepsilon_0} - z_\sigma} \right)^{\sigma - 1} \frac{\exp(\beta\varepsilon_0 - F_\sigma^{(0)} - \sigma)}{(\sigma - 1)!},$$

differing again by universal renormalization factors

$$R_\sigma = \sqrt{2\pi\sigma}\,\sigma^{\sigma-1} e^{-\sigma}/(\sigma - 1)!$$

from the results provided by the standard saddle-point scheme. Stirling's formula for $(\sigma - 1)!$ now implies $R_\sigma \to 1$ for large σ: The incorrect standard scheme becomes *better* when the order σ of the ground-state pole is *increased*. This seemingly paradoxical result — after all, it is the ground-state pole which spoils the standard scheme — finds its explanation in the saddle-point equation (13): In a system with a σ-fold degenerate ground state, each individual state takes only $(1/\sigma)$-th of the population that a non-degenerate state would have to carry. Therefore, the distance from $e^{\beta\varepsilon_0}$ to the saddle point z_σ is of the order $O(\sigma/N)$, so that increasing σ drives z_σ away from the singular point, thereby lessening the error.

If one naively uses the standard scheme for evaluating condensate fluctuations, disaster strikes: Then the ''approximations'' to the three terms on the right-hand side of Eq. (14) are off by factors R_1/R_2, $(R_1/R_2)^2$, and R_1/R_3, respectively, wrongly suggesting that $\langle \delta^2 n_0 \rangle_{\mathrm{cn}}$ does not vanish properly for $T \to 0$, but rather approaches $0.02438N^2$ — which, for large N, is huge. In contrast, our amended scheme works with utmost accuracy. Figure 3 shows the rms fluctua-

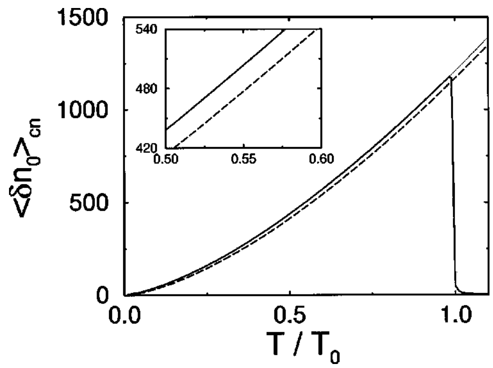

FIG. 3. Heavy full line: Canonical rms fluctuation of the ground-state occupation number for a gas of 10^6 ideal Bosons in an isotropic harmonic trap, computed with the amended saddle-point method. The dashed line corresponds to only the leading term of the approximation (15); the thin line, visible only in the upper right corner, to the full Eq. (15). Even in the inset, the heavy and the thin line remain indistinguishable.

tion $\langle \delta n_0 \rangle_{\rm cn} \equiv \langle \delta^2 n_0 \rangle_{\rm cn}^{1/2}$ for 10^6 ideal Bosons in an isotropic trap, and compares the saddle-point result to the approximation

$$\langle \delta^2 n_0 \rangle_{\rm cn} = \tau^3 \zeta(2) + \tau^2 (1.5 \ln \tau + 3.7608) - 0.5\tau \quad (15)$$

with $\tau = k_B T/(\hbar\omega) \gg 1$, which can be derived under the assumption of an infinite reservoir of condensate particles for this particularly simple trap [6,14]. The strength of the saddle-point approach, of course, lies in the fact that it works with the same simplicity also for every other trap geometry, and that it can easily be adapted to the microcanonical ensemble [13].

Experimentally realized condensates in harmonic traps are weakly interacting, i.e., they satisfy $N(a/L)^3 \ll 1$, where a is the s-wave scattering length of the atomic species with mass m and $L = \sqrt{\hbar/(m\omega)}$. In addition, one usually has $Na/L \gg 1$, placing the system in the Bogoliubov regime [15]. Spin-polarized hydrogen atoms [16], with their rather low scattering length $a = 0.0648$ nm [17], form an exception that comes closer to the ideal gas: Taking a shallow trap with $\omega = 100\ \mathrm{s}^{-1}$, one has $Na/L \approx 1$ even for $N = 400\,000$. Thus, it is possible to prepare systems intermediate between the ideal gas and the Bogoliubov gas. If one assumes the validity of first-order perturbation theory, the partition function of such a very weakly interacting gas can be expressed in terms of partition functions of ideal gases [4,18]. Hence, for exploring the non-trivial crossover [15] from the ideal gas to the Bogoliubov gas, the techniques sketched here should prove invaluable.

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